Thioacetamide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.22 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.76e-01

Confidence level: 7.25e-01

Nearest Neighbors from the Training Set

Image not found
Thioacetamide
Measured: 2.17
Predicted: 4.22

Image not found
Allylamine
Measured: 17.5
Predicted: 17.5

Image not found
Furfurylamine
Measured: 10.3
Predicted: 12.4

Image not found
Ethanamine
Measured: 22.2
Predicted: 21.1

Image not found
Propylamine
Measured: 16.9
Predicted: 17.1